Roughness Scaling of Deconstruction Interfaces.

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Abstract

The scaling properties of one-dimensional deconstructed surfaces are studied by numerical simulations of a disaggregation model. The model presented here for the disaggregation process takes into account the possibility of having quenched disorder in the bulk under deconstruction. The disorder can be considered to model several types of irregularities appearing in real materials (dislocations, impurities). The presence of irregularities makes the intensity of the attack to be not uniform. In order to include this effect, the computational bulk is considered to be composed by two types of particles. Those particles which can be easily detached and other particles that are not sensible to the etching attack. As the detachment of particles proceeds in time, the dynamical properties of the rough interface are studied. The resulting one-dimensional surface show self-affine properties and the values of the scaling exponents are reported when the interface is still moving near the depinning transition. According to the scaling exponents presented here, the model must be considered to belong to a new universality class.

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1 Introduction

There are three fundamental physical processes that gives rise to the morphology of a surface: deposition, surface diffusion and desorption. In the past decade, the characteristics of the interfaces generated by the combination of deposition and surface diffusion has been well studied. [1, 2, 3] In particular for growth models, particles are added to the surface and then they are allowed to relax by different mechanisms. Many of this models have been shown to lead to the formation of self-affine surfaces, characterized by scaling exponents. From a theoretical point of view, the studies dedicated to the self-affine interfaces generated by growth models can be considered to follow two main branches. The studies about the properties of discrete models and the studies about continuous models. Discrete models where dedicated mainly to the study of the properties of computational models in which the growth proceeds on an initially empty lattice representing a d-dimensional substrate. At each time step, the height of the lattice sites is increased by units (usually one unit) representing the incoming particles. Different models only differs on the relaxation mechanisms proposed to capture specific experimental characteristics. Then, the models are classified according to the values of the scaling exponents in several universality classes. The continuous models, [4] on the other hand, are based on stochastic differential equations of the type

$$\partial h/\partial t = F - \nabla . \, \mathbf{j} + noise \, , \tag{1}$$

in which $h(\mathbf{r}, t)$ is the thickness of the film deposited onto the surface during time t, F denotes the deposition rate and $\mathbf{j}$ denotes the current along the surface which in turn depends on the local surface configuration. If the surface current $\mathbf{j}$ represents some experimental nonlinear equilibrium processes it may gives rise to different types of nonlinear terms. The *noise* term corresponds to the fluctuations in the growth rate and, in general, is assumed to be uncorrelated. The differential equations are solved, either numerically or analytically (when it is possible), and the scaling exponents are determined. If the values of the exponents are similar to those of the discrete models, it is said that both (discrete and continuous models) belong to the same universality class. Although, the formal connection between both approaches (discrete and continuous) is still an open question.

Other type of models in which the interface shows dynamic scaling properties are those related with fluid invasion in porous media. In this case, the noise term in Eq. 1 takes the form $\eta(\mathbf{r}, h(\mathbf{r}, t))$, which is

known as *quenched noise* and is considered to be uncorrelated. Usually, the corresponding discrete computational models resume all kind of irregularities that a appear in real porous media by invading a computational porous media which has only blocked and non-blocked sites. These models are classified according to its own universality classes in the same way that others growth models.

Desorption or detaching processes, despite its technological importance, have not received the same amount of attention. Maybe because they were considered to be, simply, the reciprocal of the growth models and no new characteristics were expected to appear.

There are many technological processes depending on the details of the etching phenomena and only recently few of them have been modeled in order to understand the phenomena at an atomic level. [5] For instance, corrosion is among the most important disaggregation processes because its economical importance. In this sense a simple deconstruction model was just introduced by Reverberi and Scalas (RS).[6] They found that their model is in fact the reciprocal of a growth model known as Wolf-Villain (WV) model,[7] and that the interface show the same characteristic exponents. In this paper we present a discrete disaggregation model, which can be considered as a generalization of the above mentioned RS deconstruction model. Besides its importance from an experimental point of view, academically, it is worth to study a deconstruction model in which the attack process may take place upon an heterogeneous material, because its ubiquity in many technological and applied areas.

2 Theory

Following previous studies realized on growth models, it is expected that the deconstructed surface will present self-affine properties. According to the rules depicted below for the computational model, no overhangs will be generated and the surface will be of the solid-on-solid (SOS) type. Then, the characteristics of interest are the scaling properties of the width (or roughness) defined as

$$\omega(L,t) = \left[\langle h^2(x,t)\rangle_x - \langle h(x,t)\rangle_x^2\right]^{1/2} \quad , \tag{2}$$

where $\langle\cdot\rangle_x$ denotes ensemble average over the entire lattice size L, $h(x,t)$ is the height (measured from the bottom) of the column at position x, $\langle h(x,t)\rangle_x$ is the average surface height and t is the time, roughly proportional to the number of removed monolayers m.

As for a growth processes we assume that the roughness obeys the Family-Vicsek scaling relation, [8] valid for SOS self-affine interfaces,

$$\omega(L,t) = L^{\alpha}\, f\left(\frac{t}{L^{z}}\right) \ , \tag{3}$$

being α the roughness exponent because $\omega \sim L^{\alpha}$ when $t \gg L^{z}$ and β the growth exponent because $\omega \sim t^{\beta}$ when $t \ll L^{z}$. Of course, in the case studied here there is no *growth*, but an exponent β can be defined in the same way. $z = \alpha/\beta$ is the dynamic exponent. From a computational point of view, there are various ways in which the scaling exponents can be calculated. The exponent β is usually determined by measuring the slope of the log-log plot of $\omega(L,t)$ vs t at early times. For the exponent α, several techniques are available. In discrete models, simulations with different systems sizes L can be made. Then the values of the saturation width, ($\omega_s = \omega(L,t)$ for $t \gg L^{z}$), are plotted against L and the exponent α is determined directly from the plot. On the other hand, the height-height correlation function defined as $c(r,\tau) = \langle [h(x,t) - h(x+r,t+\tau)]^2 \rangle^{1/2}$, can be used. The correlation function is known to scale in the same way as the width $w(L,t)$; in particular for $t \gg L^{z}$ and for $r \ll L$ the correlation function behaves as $c(r,0) \sim r^{\alpha}$. A third technique for calculating the dynamic exponent α is based in the scaling properties of the structure factor. [3] Within this approach the dynamic scaling behavior can be investigated by calculating the structure factor (power spectrum) defined as

$$S(k,t) = \langle h(k,t) h(-k,t) \rangle \quad , \tag{4}$$

where $h(k,t) = (L^{-1/2}) \sum_x [h(x,t) - \overline{h(t)}] e^{ikx}$. The structure factor scales as

$$S(k,t) = k^{-(2\alpha+1)} g(t/k^{-z}) \ , \tag{5}$$

where the scaling function has the form

$$g(u) = \begin{cases} u^{(2\alpha+1)/z} & u \ll 1 \ , \\ const & u \gg 1 \ . \end{cases} \tag{6}$$

The equation $\omega^2(L,t) = (1/L) \sum_k S(k,t)$ gives the relation between the roughness and the structure factor. [2]

[2]Recently, [11] a generalization of the scaling properties of S(k,t) has been proposed. However here it is considered that the Family-Vicsek scaling anzat is obeyed and hence the scaling properties of the structure factor must be those represented by equations (5-6).

It is worth to mention that for $t \gg L^z$, the structure factor does not show any dependence with the lattice size L. This characteristic makes $S(k)$ very suitable to calculate the exponent α using smaller system sizes for the simulations. This approach will be used here.

3 Computational Model

As stated above, the deconstruction model presented by Reverberi and Scalas can be considered as the reciprocal of the WV growth model and shows the same values of the scaling exponents. In the RS model the deconstruction proceeds by picking at random a site in the lattice and remove the particle which presents the smaller amount of bonds between the selected one and its nearest neighbors. On the other hand, in the WV model the deposition process is as follows; after selecting at random a site, the number of bonds of the site is calculated as well as the number of bonds of it nearest neighbors sites. The particle is deposited in the site with the larger amount of bonds. This deposition mechanism is justified by saying that the number of bonds of a site is *roughly* proportional to the *local chemical potential*, because the number of bonds increases with the local curvature of the interface, i.e., $\mu(x,t) \propto -\nabla^2 h(x,t)$. In this sense, another growth model can be formulated. This model is called the *larger curvature* (LC) model and was introduced by Kim and Das Sarma. [9] In this case, the larger local curvature $[h(x+1) + h(x-1) - 2h(x)]$ between a random selected site and its neighbors is used to decide where to deposit the new incoming particle. It can be shown, by using an argument based on a Hamiltonian, that the LC model belongs to the same universality class that the WV model. [9]

Following this line of reasoning, a deconstruction model equivalent to the RV model would be one in which particles are removed from the site with the *smaller* value of the local curvature. This would be the reciprocal of the LC growth model. Lets call it the *smaller curvature* (SC) deconstruction model. Of course, by the same arguments stated above, the RV and the SC deconstruction models will belong to the same universality class; the WV and LC universality class.

The model presented here is mostly related with another type of growth models. Those in which the advance of the interface takes place on a random environment.[3] Several models of this kind has

[3]However, as it is shown below, the model presented here is not the direct reciprocal

been presented and their universality classes and scaling exponents has been studied. [2, 3] In those models, the growing interface advances in a random environment. Usually, the randomness of a real porous media is resumed in a computational random media in which there are a certain amount of sites which are blocked to the advance of the interface while others are not. [3, 10] Beyond a certain amount of blocked sites present in the system the interface becomes *pinned* and cannot advance any more. The scaling properties of such interfaces is, in general, studied near the pinning transition.

Here, and in order to model various types of real heterogeneities, the deconstruction is considered to take place on a bulk in which two types of particles are present, those particles susceptible to the etching and those which cannot be detached by the external agent acting upon the interface. Then, the deconstruction rules run as follows. A surface is represented by a one-dimensional array of integers specifying the number of atoms in each one of the columns of the bulk. To maintain the solid-on-solid characteristic of the model, the detaching processes will not give rise to overhangs. Each column of the one-dimensional array (indexed by i) is initially filled enough in order to allow the deconstruction process to take place during the whole simulational time, i.e., no column height must become negative at the end of the simulation. Before starting the deconstruction, at each lattice site $[i, h(i)]$ a particle of the type A is placed with probability $(1 - P)$ and a particle of type B is placed with probability P. Particles A are considered to be susceptible to the attack, while particles B no. Initially all columns are filled with the same amount of atoms, so the the simulations start with a flat surface at $t = 0$. The selectivity of the deconstruction process is simulated in the following way. A column K is picked at random. The local curvature $[h_{i+1} + h_{i-1} - 2h_i]$ is calculated for $i = K$, $i = K+1$ and $i = K-1$. The particle at the top of the column with the *smaller* curvature is removed ($h_K \to h_K - 1$) if it is of type A, otherwise it is not removed. However, if the local curvature is smaller than a certain threshold θ the particle is removed, no matter which type it is. [4] A value of $\theta = -1$ and periodic boundary conditions were used. It is worth to notice that for P=0, i.e., just

of any of the known growth models.

[4] In this way, the possibility of *lateral* attack is taken into account. For instance, it could happen that a particle B may remain at the top of a long column. In a real situation, lateral attack could detach A particles underneath, leaving particle B isolated from the interface.

particles of type A in the system, the model turns to be the SC model, the reciprocal of the LC model.

4 Results and Discussion

Main results are summarized by the plots presented in Figs.1 and 2. In both figures, ensemble averages where taken over 500 independent runs. A value of $L = 2^{11}$ was used in Fig.1, while $L = 2^9$ was used in Fig.2. As it was numerically tested, there is a critical probability that pinn the interface at $P = P_c \cong 0.14$. A value of P slightly under P_c, $P = 0.13$, was used in order to study the properties of the interface near the pinning transition. It is worth to notice that the critical probability has a different value than those corresponding to the directed percolation transition, which is the effect responsible of the pinning transition in interfaces invading porous media. It can be thought that the difference is due to the fact that, in the model presented here, the interface becomes pinned when *two* simultaneous conditions are fulfilled: the local curvature is greater than θ *and* all the particles at the interface are of type B. On the other hand, in growth models on porous media it is enough to have a lateral directed percolation effect in order to pinn the interface.

In Fig.1, values of the exponent β as a function of time are presented. The figure was constructed by calculating, at each time t, the slope of the roughness as $[log(w_{t+\Delta t}) - log(w_t)]/\Delta t$. In particular, $\Delta t = 10$ was used. This method for determining the exponent β is known as the *consecutive slopes* method. [3] It can be seen that the calculated values fluctuate between 0.6 and 0.7 for the first 1000 layers removed. The average value of the exponent calculated up to $t = 1000$ is $\beta = 0.676$. For comparison, the corresponding exponent for the advance of an interface in porous media was found to be $\beta = 0.7$. [10]

In Fig.2 the a plot of the structure factor $S(k)$ is shown. As stated above, for $t \gg L^z$ the structure factor behaves has $S(k) \sim k^\gamma$ with $\gamma = 2\alpha + 1$. The slope of a line trough the points was found to be -3.27 ± 0.0085, which gives a value of $\alpha \cong 1.135$. In this case the value of the exponent is quite different from the corresponding to interfaces advancing in porous media, $\alpha = 0.7$. [10]

The values of α and β indicate that the exponent z is $z = \alpha/\beta \cong 1.8$ and that the scaling relation $\alpha + z = 2$ is not fulfilled. Although, due to the strong nonlinear effects present in the evolution of the interface, it is not expected to hold.

Final, it is pointed out that same kind of simulations were done using $P = 0.0$. In this case the disorder in the bulk has no influence, since there are just one type of particles in the system. Then the model is equivalent to the SC or the RV models, which in turn are the reciprocal of the LC or WV models. The equivalence is confirmed by the values of the exponents obtained for the no-disorder case: $\beta = 0.353$ and $\alpha = 1.385$, in good agreement with the previously reported values, $\beta = 0.365$ and $\alpha = 1.4$, for the WV model. [7]

5 Conclusions

A new deconstruction model has been presented. In the model the natural heterogeneities present in all materials of technological relevance were include. According to the values obtained for the scaling exponents the model could be though to belong to a new universality class, when the properties of the interface are studied near the pinning transition. The values of the exponents indicate that there is no growth model which can be associated as the reciprocal of the model analyzed here. In this sense a theoretical continuum model need to be developed. As a natural continuation of the present work, simulations on higher dimensions are under development.

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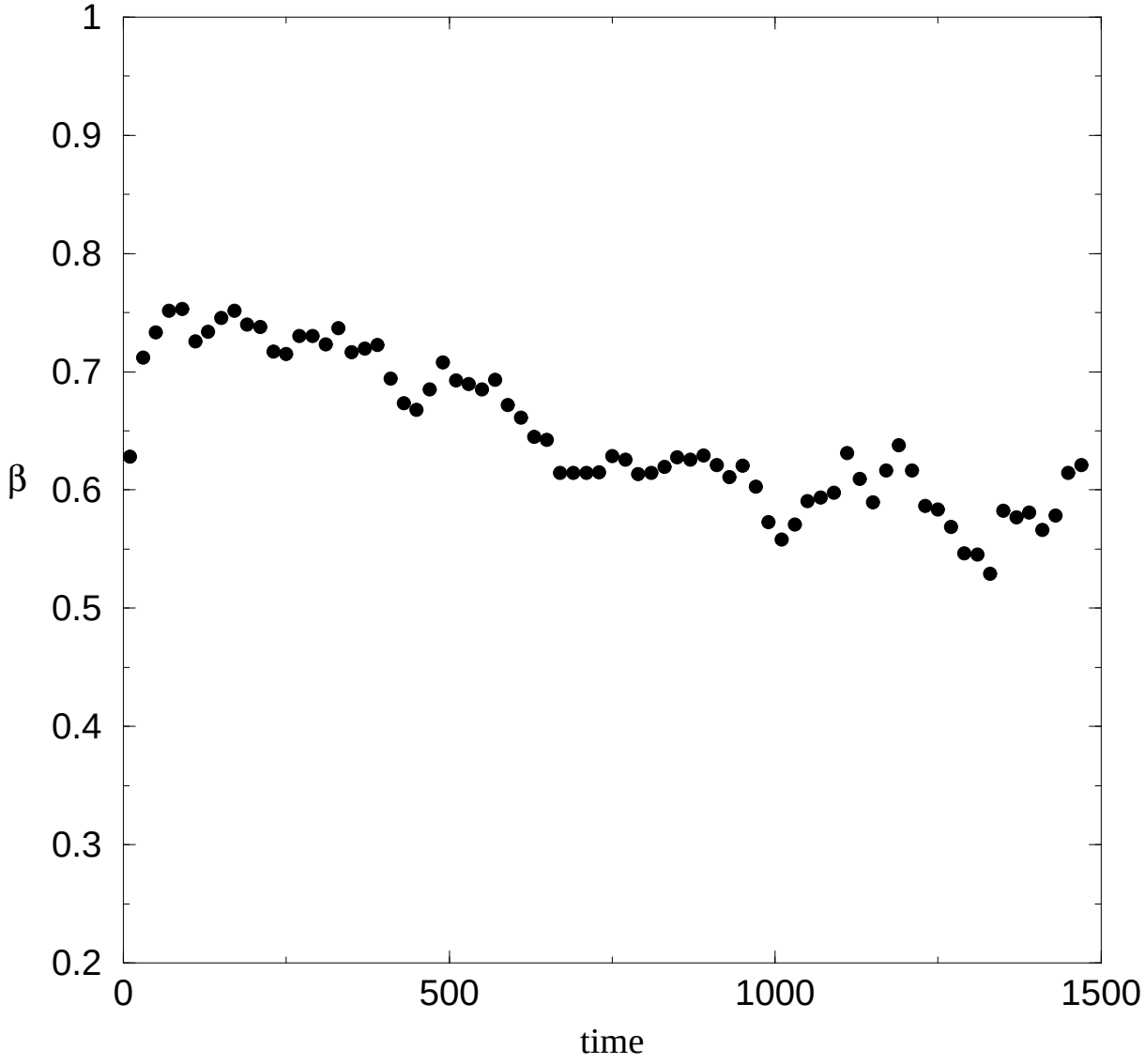

Figure 1: Values of the exponent β as a function of time. The average value, between $t = 100$ and $t = 1000$ is 0.676. Values of $L = 2^{11}$ and $P = 0.13$ were used.

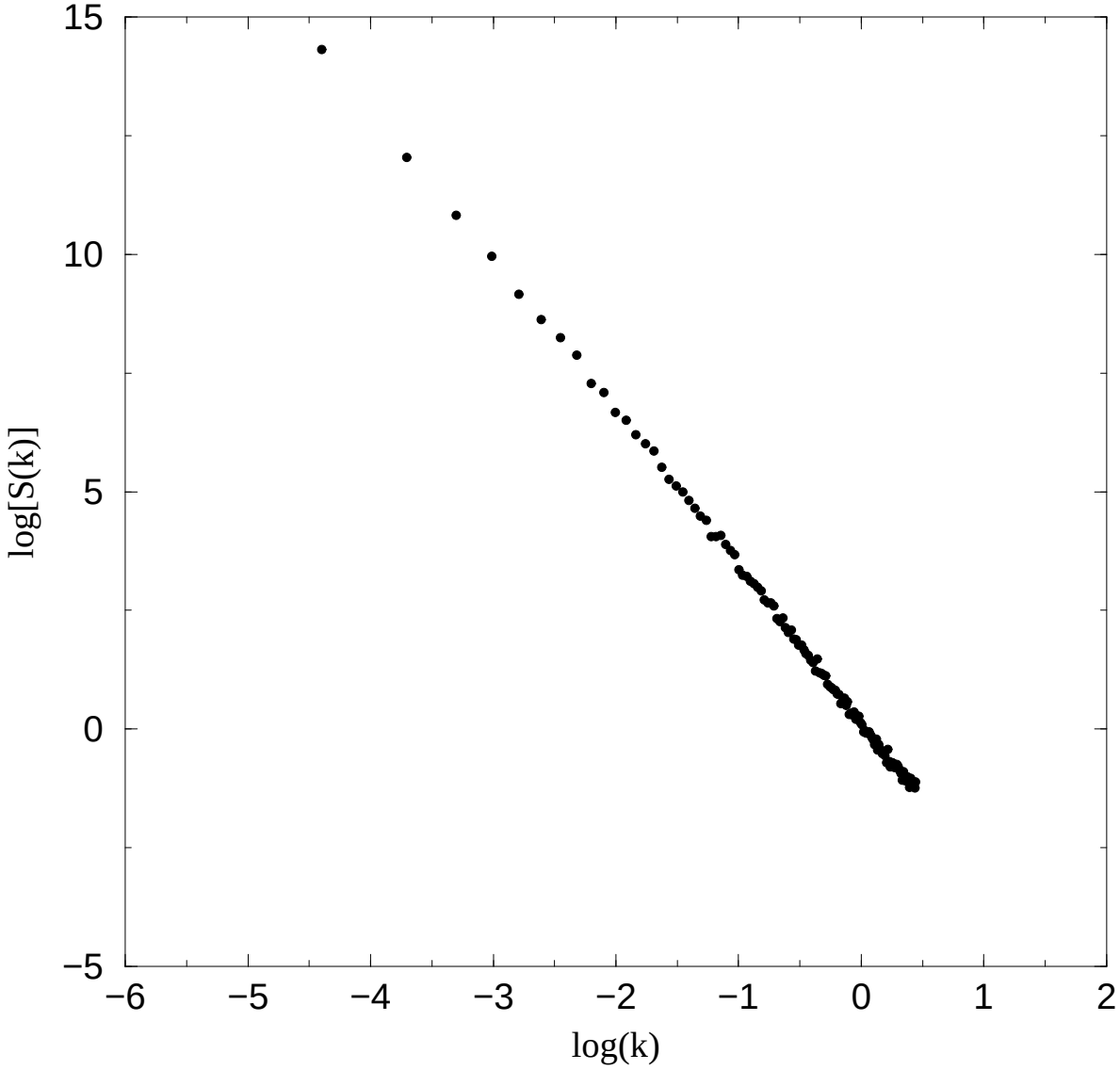

Figure 2: Plot of the structure factor $S(k)$ for $t \gg L^z$ and $L = 2^9$, with $P = 0.13$. The slope of a line through the points is $\gamma = -3.27 \pm 0.0085$.

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